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**Molecular Dynamics Simulations of Microphase Separating Tapered Diblock Copolymers** YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — Tapered AB copolymers consist of pure A and B blocks separated by a middle, random block whose average composition is a linear gradient from pure A to pure B (or from B to A for an inverse taper). These systems microphase separate into ordered structures similar to typical AB diblock copolymers. Prior experiments and theory suggest that one can use taper length as an adjustable parameter (beyond those available in the diblock system) to control interfacial and phase behavior, and that tapers potentially make the bicontinuous double gyroid phase more accessible at high molecular weight. Using a simple bead-spring model, we perform molecular dynamics (MD) simulations to determine the interfacial profiles and other features of the structure and dynamics as a function of taper length. The pairwise interactions are purely repulsive with stronger A-B than A-A or B-B repulsions. We find increasing the taper length increases miscibility and widens the interfacial region. The change in the interfacial density profile with taper length is similar to that from self-consistent field theory (SCFT) and fluids density functional theory (fDFT). A detailed comparison between the microphase separated structures obtained from MD, SCFT, and fDFT will be presented.

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